

NORMAN-SLE:

Unleashing the Power of Chemical Data Beyond FAIR

LCSB



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26 October 2023

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

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Search

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WELCOME TO THE NORMAN NETWORK

The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. It specifically seeks both to promote and to benefit from the synergies between research teams from different countries in the field of emerging substances.

Who should be part of the network?

All interested stakeholders dealing with emerging substances – whether in studying their occurrence and effects or risk assessment and risk management:

- » Competent authorities / Reference laboratories: i.e. institutes and organisations designated by the competent authorities at the national level to offer technical and scientific support in specific fields related to environmental protection.
- » Research centres and academia.
- » Industry stakeholders.
- » Government institutions and standardisation bodies.

Are you involved in research on the occurrence and environmental effects of emerging substances? Or are you concerned with the assessment and management of the risks associated with them? If so, you are a potential stakeholder in the NORMAN network.

If you are interested in this initiative, which has attracted a membership of more than 80 leading laboratories and authorities across Europe, North America and Asia, please contact:

Ms. Valeria DULIO,
Executive Secretary of the NORMAN network
INERIS, Direction Scientifique
Rue Jacques Taffanel – Parc Technologique ALATA
F-60550 Verneuil-en-Halatte,
E-mail address: valeria.dulio@ineris.fr

[Read more](#)

WG1: Prioritisation
WG2: Bioassays
WG3: EDA
WG4: Nano-and micro scale particulate contaminants
WG5: Water reuse and policy support
WG6: Emerging substances in the indoor environment
WG7: Contaminants of emerging concern in soil and the terrestrial environment
WG8: Marine environment
Cross-Working Group Activity: Passive sampling
Cross-Working Group Activity Non-target Screening (NTS)

The screenshot shows the NORMAN Database System homepage. At the top, the NORMAN logo is centered above the title "NORMAN Database System". Below the title, a short paragraph states: "NORMAN organises the development and maintenance of various web-based databases for the collection & evaluation of data / information on emerging substances in the environment". The main content area is a grid of 12 database modules, each with an icon, a title, and a brief description. Two modules, "Suspect List Exchange" and "MassBank Europe", are highlighted with red rectangular boxes. The "Suspect List Exchange" module includes a small profile picture of a woman. The "MassBank Europe" module includes a small profile picture of a woman. The modules are arranged in three columns and four rows.

SEARCH All Databases
Searching for individual substance or group(s) of substances in all databases
Note: Click on a link below to go to an individual database home page

Substance Database
A merged list of NORMAN substances; Central Database to access various lists of substances for suspect screening and prioritisation

Suspect List Exchange
Central Database to access various lists of substances for suspect screening and prioritisation

Digital Sample Freezing Platform
A database of mass chromatograms obtained by LC-HR-MS for retrospective screening of environmental samples

Substance Factsheets
A summary information on individual substances from all NORMAN Database System modules

Chemical Occurrence Data
A database of geo-referenced monitoring data on emerging substances

Antibiotic Resistance Bacteria/Genes
A database of ARBs/ARGs in environmental matrices

Indoor Environment
A database of data in indoor environment matrices

Prioritisation
Results of prioritisation of NORMAN substances using the NORMAN Prioritisation Framework

SARS-CoV-2 in sewage
A database with the latest information on SARS-CoV-2 in sewage across Europe and internationally; including a common protocol for sample collection, storage, extraction, analysis and data sharing to support the development of an international comparable data set.

Ecotoxicology
A platform for systematic collection and evaluation of ecotoxicity studies for harmonised derivation of environmental quality standards

MassBank Europe
A database of mass spectra of emerging substances to support identification of unknown substances

Passive Sampling
A database of data obtained with passive samplers

Bioassays Monitoring Data
A database of data obtained by analysis of environmental samples with bioassays

NORMAN-SLE : Gathering Expert Info



🏠 NORMAN WEBSITE | 🗄️ NORMAN DATABASE SYSTEM | 🏠 HOME | 👤 LOGIN

NORMAN SUBSTANCE DATABASE

NORMAN Suspect List Exchange – NORMAN SLE

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring questions. The NORMAN-SLE documents all individual collections that form a part of the merged collection [NORMAN SusDat](#). The original SLE lists should be consulted to verify SusDat information if necessary (see Source column in SusDat). NORMAN-SLE versions are tracked on [Zenodo](#).

Comments and contributions are welcome - please email us at suspects@normandata.eu.

Please refer to our [documentation](#) pages for: [citation](#) instructions, [credits](#), [updates](#), [license](#) details, [SDFs](#) and other useful tips!

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S0	SUSDAT	Merged NORMAN Suspect List: SusDat	Interactive Data table SusDat with Haz and Expo scores as XLSX , CSV (18/01/2022) MetFrag CSV (03/03/2020) CompTox SUSDAT List	SusDat InChIKeys: All , MS-ready (18/01/2022)	A merged list of >111,000 structures from SLE suspect lists. See interactive version . Compiled by Reza Aalizadeh, Nikiforos Alygizakis and Lubos Cirka, University of Athens/EI, including RTI and toxicity values, with Hazard and Exposure values provided by Stellan Fischer, KEMI, documented here . <i>Work in progress ... please report any issues!</i> DOI: 10.5281/zenodo.2664077

NORMAN-SLE : Gathering Expert Info



NORMAN Suspect List Exchange – NORMAN SLE

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN questions. The NORMAN-SLE documents all individual collections that form a part of the merged collection NORMAN (see Source column in SusDat). NORMAN-SLE versions are tracked on [Zenodo](#).

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No.	Abbreviation	Description	Link to full list
S0	SUSDAT	Merged NORMAN Suspect List: SusDat	Interactive Data table SusDat with Haz and Expo scores as XLSX , CSV (18/01/2020) MetFrag CSV (03/03/2020) CompTox SUSDAT List

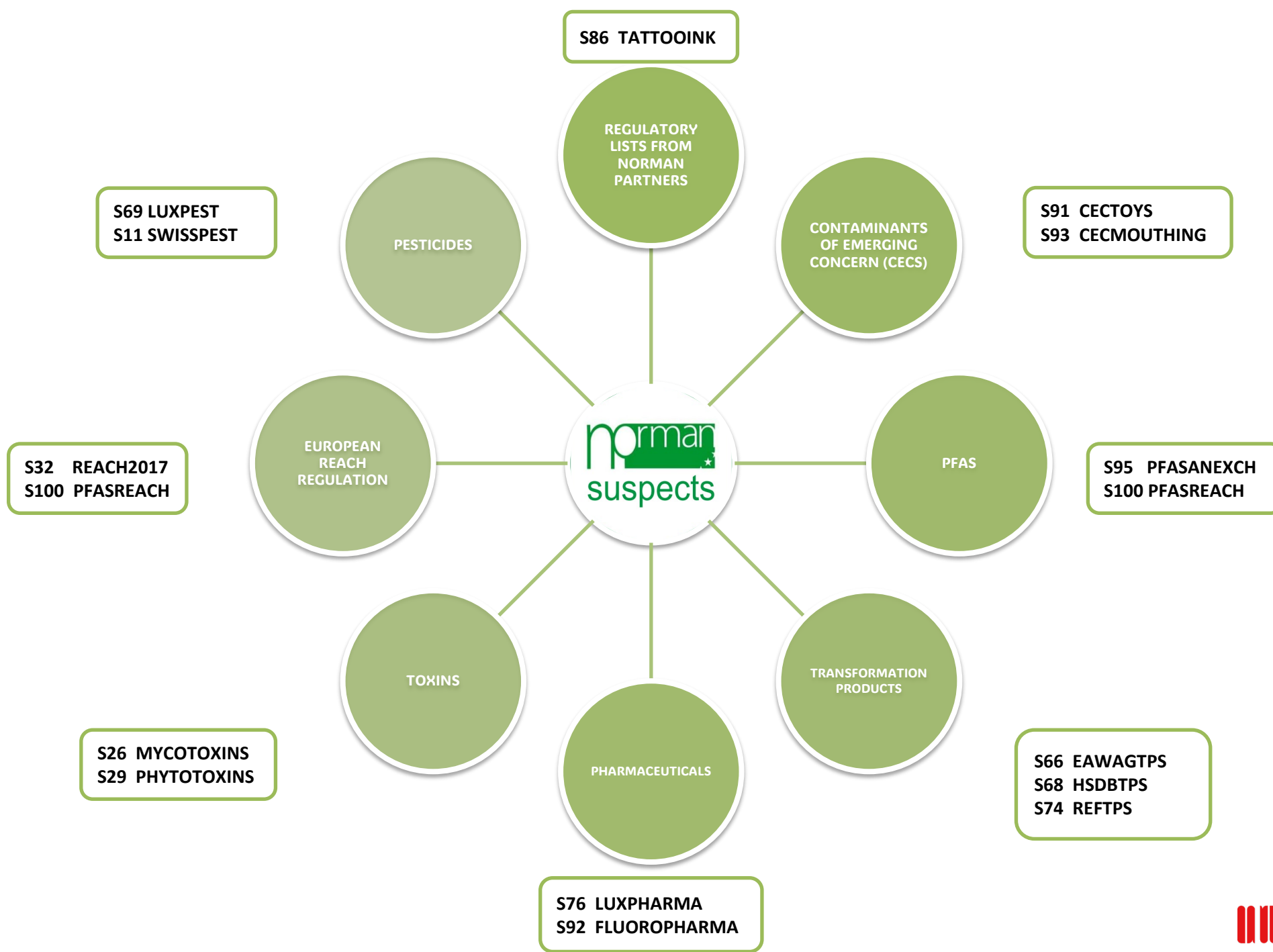
RESEARCH

Open Access



The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

Hiba Mohammed Taha¹, Reza Aalizadeh², Nikiforos Alygizakis^{3,2}, Jean-Philippe Antignac⁴, Hans Peter H. Arp^{5,6}, Richard Bade⁷, Nancy Baker⁸, Lidia Belova⁹, Lubertus Bijlsma¹⁰, Evan E. Bolton¹¹, Werner Brack^{12,13}, Alberto Celma^{10,14}, Wen-Ling Chen¹⁵, Tiejun Cheng¹¹, Parviel Chirsir¹, Ľuboš Čirka^{16,3}, Lisa A. D'Agostino¹⁷, Yannick Djoumbou Feunang¹⁸, Valeria Dulio¹⁹, Stellan Fischer²⁰, Pablo Gago-Ferrero²¹, Aikaterini Galani², Birgit Geueke²², Natalia Glowacka³, Juliane Glüge²³, Ksenia Groh²⁴, Sylvia Grosse²⁵, Peter Haglund²⁶, Pertti J. Hakkinen¹¹, Sarah E. Hale⁵, Felix Hernandez¹⁰, Elisabeth M.-L. Janssen²⁴, Tim Jonkers²⁷, Karin Kiefer²⁴, Michal Kirchner²⁸, Jan Koschorreck²⁹, Martin Krauss¹², Jessy Krier¹, Marja H. Lamoree²⁷, Marion Letzel³⁰, Thomas Letzel³¹, Qingliang Li¹¹, James Little³², Yanna Liu³³, David M. Lunderberg^{34,35}, Jonathan W. Martin¹⁷, Andrew D. McEachran³⁶, John A. McLean³⁷, Christiane Meier²⁹, Jeroen Meijer³⁸, Frank Menger¹⁴, Carla Merino^{39,40}, Jane Muncke²², Matthias Muschket¹², Michael Neumann²⁹, Vanessa Neveu⁴¹, Kelsey Ng^{3,42}, Herbert Oberacher⁴³, Jake O'Brien⁷, Peter Oswald³, Martina Oswaldova³, Jaqueline A. Picache³⁷, Cristina Postigo^{44,14}, Noelia Ramirez^{45,39}, Thorsten Reemtsma¹², Justin Renaud⁴⁶, Pawel Rostkowski⁴⁷, Heinz Rüdell⁴⁸, Reza M. Salek⁴¹, Saer Samanipour⁴⁹, Martin Scherlinger^{23,42}, Ivo Schliebner²⁹, Wolfgang Schulz⁵⁰, Tobias Schulze¹², Manfred Sengli³⁰, Benjamin A. Shoemaker¹¹, Kerry Sims⁵¹, Heinz Singer²⁴, Randolph R. Singh^{1,52}, Mark Sumarah⁴⁶, Paul A. Thiessen¹¹, Kevin V. Thomas⁷, Sonia Torres³⁹, Xenia Trier⁵³, Annemarie P. van Wezel⁵⁴, Roel C. H. Vermeulen³⁸, Jelle J. Vlaanderen³⁸, Peter C. von der Ohe²⁹, Zhanyun Wang⁵⁵, Antony J. Williams⁵⁶, Egon L. Willighagen⁵⁷, David S. Wishart⁵⁸, Jian Zhang¹¹, Nikolaos S. Thomaidis², Juliane Hollender^{23,24}, Jaroslav Slobodnik³ and Emma L. Schymanski¹



NORMAN-SLE WORKFLOW

Suspect List(s)

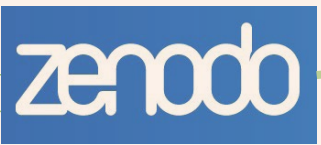
Name	Preferred_Name	InChIKey	IUPAC_Name	SMILES	InChI	Molecular_Formula	Monoisotopic_Mass	PubChem_CID
Cypermethrin	Cypermethrin	KAATUXN	Cyano(3-pher	CC1(C)C(C	InChI=1S/	C22H19Cl2NO3	415.0741989	2912
Difenacoum	Difenacoum	FVQITOLC	3-[3-([1,1'-Bip	OC1=C(C2	InChI=1S/	C31H24O3	444.1725446	54676884
Flocoumafen	Flocoumafen	KKBGNYHI	4-Hydroxy-3-[OC1=C(C2	InChI=1S/	C33H25F3O4	542.1704938	54698175
Permethrin	Permethrin	RLLPVAHG	(3-Phenoxy)pl	CC1(C)C(C	InChI=1S/	C21H20Cl2O3	390.0789499	40326
Dimethyltolylsulfamid	N,N-Dimethyl-N'-p-t	UDCDOJQ	N,N-Dimethy	CN(C)S(=C	InChI=1S/	C9H14N2O2S	214.0775989	738302
Dimethylsulfamid	Sulfamide, N,N-dim	QMHAHU	N,N-Dimethy	CN(C)S(N)	InChI=1S/	C2H8N2O2S	124.0306487	134472
Ethylenharnstoff	Ethylene urea	YAMHXTC	Imidazolidin-	O=C1NCC	InChI=1S/	C3H6N2O	86.04801282	8453
Ethylenthioharnstoff	Ethylene thiourea	PDQAZBW	Imidazolidine	S=C1NCC	InChI=1S/	C3H6N2S	102.0251694	2723650
Chlorocresol	4-Chloro-3-methylp	CFKMVGJ	4-Chloro-3-m	CC1=C(Cl)	InChI=1S/	C7H7ClO	142.0185425	1732
Clothianidin	Clothianidin	PGOOBEC	N-[(2-Chloro-	CN\C(NCC	InChI=1S/	C6H8ClN5O2S	249.0087234	213027
Cyromazin	Cyromazine	LVQDKIWI	N~2~-Cyclopr	NC1=NC(N	InChI=1S/	C6H10N6	166.0966943	47866
Melamin	Melamine	JDSHMPZF	1,3,5-Triazine	NC1=NC(N	InChI=1S/	C3H6N6	126.0653942	7955
Diclosan	Soneclosan	BYNQFCJC	5-Chloro-2-(4	OC1=C(OC	InChI=1S/	C12H8Cl2O2	253.9901349	18807

Suspect List(s)

Eawag_ID	Name	CAS	Protected(logDpH7)	SMILES	InChi	InChiKey	MolecularExactMass
249	N4-Acetyl	127-76-4	CAS_RN:12	0.69 CC(=O)NC1=CC=CC=C1	NC1=CC=CC=C1C(=O)N	C1=CC=C(C=C1)C(=O)N	297.0242
236	4-Acetamid	83-15-8	CAS_RN:83	0.15 CC(=O)Nc1ccc(C)cc1	CC(=O)Nc1ccc(C)cc1	CC(=O)Nc1ccc(C)cc1	245.1164
245	N4-Acetyl	24341-30-8	CAS_RN:24	1 COC1=CC(C=CC1)N	COC1=CC(C=CC1)N	COC1=CC(C=CC1)N	352.0841
247	N4-Acetyl	100-90-3	CAS_RN:10	0.41 CC(=O)Nc1ccc(C)cc1	CC(=O)Nc1ccc(C)cc1	CC(=O)Nc1ccc(C)cc1	320.0943

BIOTID0000	acetaminol	1983	RZVAJINKF	InChi=15/CYP1A2; CYP2D6
BIOTID0000 <td>piroline</td> <td>1958</td> <td>QVMDECO</td> <td>InChi=15/CYP2D6</td>	piroline	1958	QVMDECO	InChi=15/CYP2D6
BIOTID0000 <td>1-(3-Trifluoromethylphenyl)ethanone</td> <td>4296</td> <td>KKIMDKM</td> <td>InChi=15/CYP2D6; CYP1A2</td>	1-(3-Trifluoromethylphenyl)ethanone	4296	KKIMDKM	InChi=15/CYP2D6; CYP1A2
BIOTID0000 <td>2-Amino-3-methylbutanoic acid</td> <td>53462</td> <td>ARZWATD</td> <td>InChi=15/CYP1A2; CYP2D6</td>	2-Amino-3-methylbutanoic acid	53462	ARZWATD	InChi=15/CYP1A2; CYP2D6

CAS Number	Name	SMILES	InChi	InChiKey	MolecularExactMass	Protected(logDpH7)	SMILES	InChi	InChiKey	MolecularExactMass																						
294	Diuron-de	BIOTID0000 (R)-haloth	118	Ethofume	BIOTID0000 (R)-haloth	4	Metamtr	BIOTID0000 (R)-3,4-Me	668	Simazine	BIOTID0000 (R)-3,4-Me	671	Terbutyl	BIOTID0000 (4R)-5-(me	672	Terbutyl	BIOTID0000 Homo-Tie	2668	Pipromi	BIOTID0000 (R)-1-(4-M	2670	Atenolol	BIOTID0000 (S)-2-(2,6	126	Methyl	BIOTID0000 (S)-2-(2,6	296	N,N-Dime	BIOTID0000 (S)-2-(2,6	3244	Betameth	BIOTID0000 (S)-2-(2,6



DOI [10.5281/zenodo.6770176](https://doi.org/10.5281/zenodo.6770176)

12,835 views

11,095 downloads

Suspect List Exchange (NORMAN-SLE)

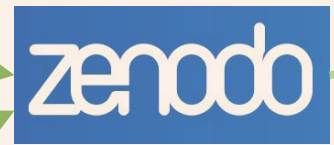
NORMAN-SLE WORKFLOW

Suspect List(s)

Eawag_ID	Name	CAS	Protected(logDpH7)	SMILES	InChi	InChiKey	MolecularExactMass
249	N4-Acetyl	127-76-4	CAS_RN:12	0.69 CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	C1=CC=C(C=C1)C(=O)N	297.0242
236	4-Acetamid	83-15-8	CAS_RN:83	0.15 CC(=O)NC1=CC=C(C=C1)	CC(=O)NC1=CC=C(C=C1)	CC(=O)NC1=CC=C(C=C1)	245.1164
245	N4-Acetyl	24341-30-8	CAS_RN:24	1 COC1=CC(C=C1)C(=O)N	COC1=CC(C=C1)C(=O)N	COC1=CC(C=C1)C(=O)N	352.0841
247	N4-Acetyl	100-90-3	CAS_RN:10	0.41 CC(=O)NC1=CC=C(C=C1)	CC(=O)NC1=CC=C(C=C1)	CC(=O)NC1=CC=C(C=C1)	320.0943

Reaction	Substrate	Enzyme	Reaction Type
BIOTID0001	acetaminol	1983 RZVAJNKFC	InChi=15/CYP1A2; CYP Oxidation
BIOTID0002	paracetamol	1983 QYMDQCI	InChi=15/CYP2A6; (m Hydroxylat
BIOTID0003	3-Trifluor	4296 KKIMDKME	InChi=15/CYP2D6; C Aromatic I
BIOTID0004	2-Amino-3	53462 ARZWATD	InChi=15/CYP1A2; C N-Hydroxy

CAS Number	Name	Priority	SMILES	InChi	InChiKey	MolecularExactMass	Substance	Enzyme	Reaction Type	Reference	DOI	DOI URL	Accession																														
294	Diuron-de	BIOTID0001	(R)-haloth	118	Ethofume	BIOTID0001	(R)-haloth	4	Metamtri	BIOTID0001	(R)-3,4-Me	668	Simazine	BIOTID0001	(R)-3,4-Me	671	Terbutylal	BIOTID0001	(4R)-5-(me	672	Terbutylal	BIOTID0001	Homo-Tie	2668	Pipromi-si	BIOTID0001	Homo-Tie	2670	Atenolol	BIOTID0001	(R)-1-(4-M	126	Methyl 2	BIOTID0001	(S)-2-(2,6	296	N,N-Dime	BIOTID0001	(2R,3S)-2-	3244	Betameth	BIOTID0001	(2R,3S)-2-



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Suspect List Exchange (NORMAN-SLE)

NORMAN-SLE WORKFLOW

NORMAN Database System (NDS)

Ecotoxicology

SARS-CoV-2 in sewage

Passive Sampling

Indoor Environment

Bioassays Monitoring Data

Digital Sample Freezing Platform

Chemical Occurrence Data

Substance Database (NORMAN SusDat)

Antibiotic Resistance Bacteria/Genes

MassBank Europe

Substance Factsheets

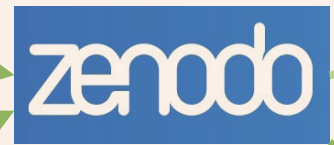
Prioritisation

Suspect List(s)

Eawag_ID	Name	CAS	Protected	logDpH7	SMILES	InChI	InChIKey	Molecular	ExactMass
249	N4-Acetyl	127-76-4	CAS_RN:12	0.69	CC(=O)NC1=CC=CC=C1	CC(=O)NC1=CC=CC=C1	C1=CC=C(C=C1)C(=O)N	133.072	133.072
236	4-Acetyl	83-15-8	CAS_RN:83	0.15	CC(=O)C1=CC=CC=C1	CC(=O)C1=CC=CC=C1	C1=CC=C(C=C1)C(=O)C	134.066	134.066
245	N4-Acetyl	24341-30-8	CAS_RN:24	1	CC(=O)NC1=CC=C(C=C1)C2=CC=CC=C2	CC(=O)NC1=CC=C(C=C1)C2=CC=CC=C2	C1=CC=C(C=C1)C(=O)NC2=CC=CC=C2	207.072	207.072
247	N4-Acetyl	100-90-3	CAS_RN:10	0.41	CC(=O)NC1=CC=C(C=C1)C2=CC=CC=C2	CC(=O)NC1=CC=C(C=C1)C2=CC=CC=C2	C1=CC=C(C=C1)C(=O)NC2=CC=CC=C2	207.072	207.072

Substrate	Substrate	Substrate	Substrate	Enzyme	Reaction
BIOTID0001	acetaminol	1983	RZVAJNKI	InChI=1S/CYP1A2; CYP2D6	Oxidation
BIOTID0001	paracetamol	1983	QYMDCCQ	InChI=1S/CYP2D6; O-aryl de	
BIOTID0001	3-Trifluoromethylphenol	4296	KKIMDKMI	InChI=1S/CYP2D6; C Aromatic 1	
BIOTID0002	2-Amino-3-methylbutanoic acid	53462	ARZWATD	InChI=1S/CYP1A2; C N-Hydroxy	

CAS Number	Name	Priority	Substance	Enzyme	Reaction	Comments
293	Diuron-de	High	Diuron	CYP1A2	Oxidation	High priority
294	Diuron-de	High	Diuron	CYP1A2	Oxidation	High priority
118	Ethofomec	High	Ethofomec	CYP1A2	Oxidation	High priority
4	Metamitri	High	Metamitri	CYP1A2	Oxidation	High priority
668	Simazine	High	Simazine	CYP1A2	Oxidation	High priority
671	Terbutyl	High	Terbutyl	CYP1A2	Oxidation	High priority
2668	Fipronil-si	High	Fipronil	CYP1A2	Oxidation	High priority
2670	Atenolol	High	Atenolol	CYP1A2	Oxidation	High priority
126	Methyl 2	High	Methyl 2	CYP1A2	Oxidation	High priority
295	N,N-Dime	High	N,N-Dime	CYP1A2	Oxidation	High priority
3244	Betameth	High	Betameth	CYP1A2	Oxidation	High priority



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Suspect List Exchange (NORMAN-SLE)

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NORMAN Suspect List Exchange Classification **115,260**

- S13 | EU-COSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) **3,887**
- S25 | OECD PFAS | List of PFAS from the OECD **3,677**

3.2.10 Collision Cross Section

150.51 Å² [M-H]⁻ [CCS Type: DT; Buffer gas: N₂; Dataset: PFAS]
DOI:10.1021/acs.est.2c00201

Baker Lab, Chemistry Department, The University of North Carolina at Chapel Hill

228.66 Å² [2M-H]⁻
150.81 Å² [M-H]⁻

S79 | UACCSECC | Collision Cross Section (CCS) Library from UAntwerp | DOI:10.5281/zenodo.4704648

NORMAN Suspect List Exchange

S80 | PFASGLUE | Overview of PFAS Uses **1,250**

NORMAN Database System (NDS)

- Ecotoxicology
- SARS-CoV-2 in sewage
- Passive Sampling
- Indoor Environment
- Bioassays Monitoring Data
- Digital Sample Freezing Platform
- Chemical Occurrence Data
- Substance Database (NORMAN SusDat)
- Antibiotic Resistance Bacteria/Genes
- MassBank Europe
- Substance Factsheets
- Prioritisation

CompTox Chemicals Dashboard

Chemical Lists

Search: NORMAN

Showing 1/4 of 300 Records

List Acronym	List Name	Chemicals	Updated	List Description
ATHENSUS	Metoprolol acid	1	2021-10-01	A compilation of suspects, predicted transformation products and surfactants for Metoprolol acid, as described in Gago-Ferreiro et al 2015, DOI: 10.1021/acs.est.5b01454. The original data is available on the NORMAN Suspect List Exchange. Status are indicated here.

7.5 Transformations

2 items View More Details

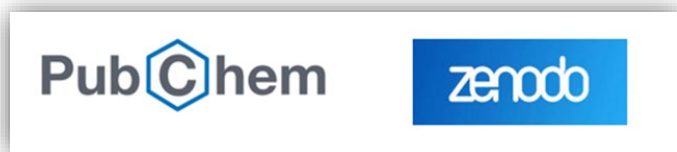
Sort By: Please Choose One

Predecessor	Predecessor Name	Successor	Successor Name	Transformation	Enzyme
	Nicotine		Norcotine	Thirdhand Smoke	
	Nicotine		Norcotine	Demethylation	

NORMAN Suspect List Exchange

NORMAN-SLE: Now >100 lists!

<https://gitlab.lcsb.uni.lu/eci/NORMAN-SLE/-/tree/master/stats#norman-sle-summary>



Stats updated Jul. 2023

Category	Number	Comment
Number of Lists	111	S00 to S111
Total Unique Compounds	115,725	From PubChem NORMAN-SLE Tree
Total Live Substances	118,557	From PubChem NORMAN-SLE Source Page
Total Live Annotations	22,335	From PubChem NORMAN-SLE Source Page
Largest List	109,631	S00 NORMAN-SusDat
Smallest List	16	S98 TIRECHEM
Total Views	86,005	From Zenodo (see below)
Unique Downloads	76,175	From Zenodo (see below)
Citations	61	From Zenodo (see below)

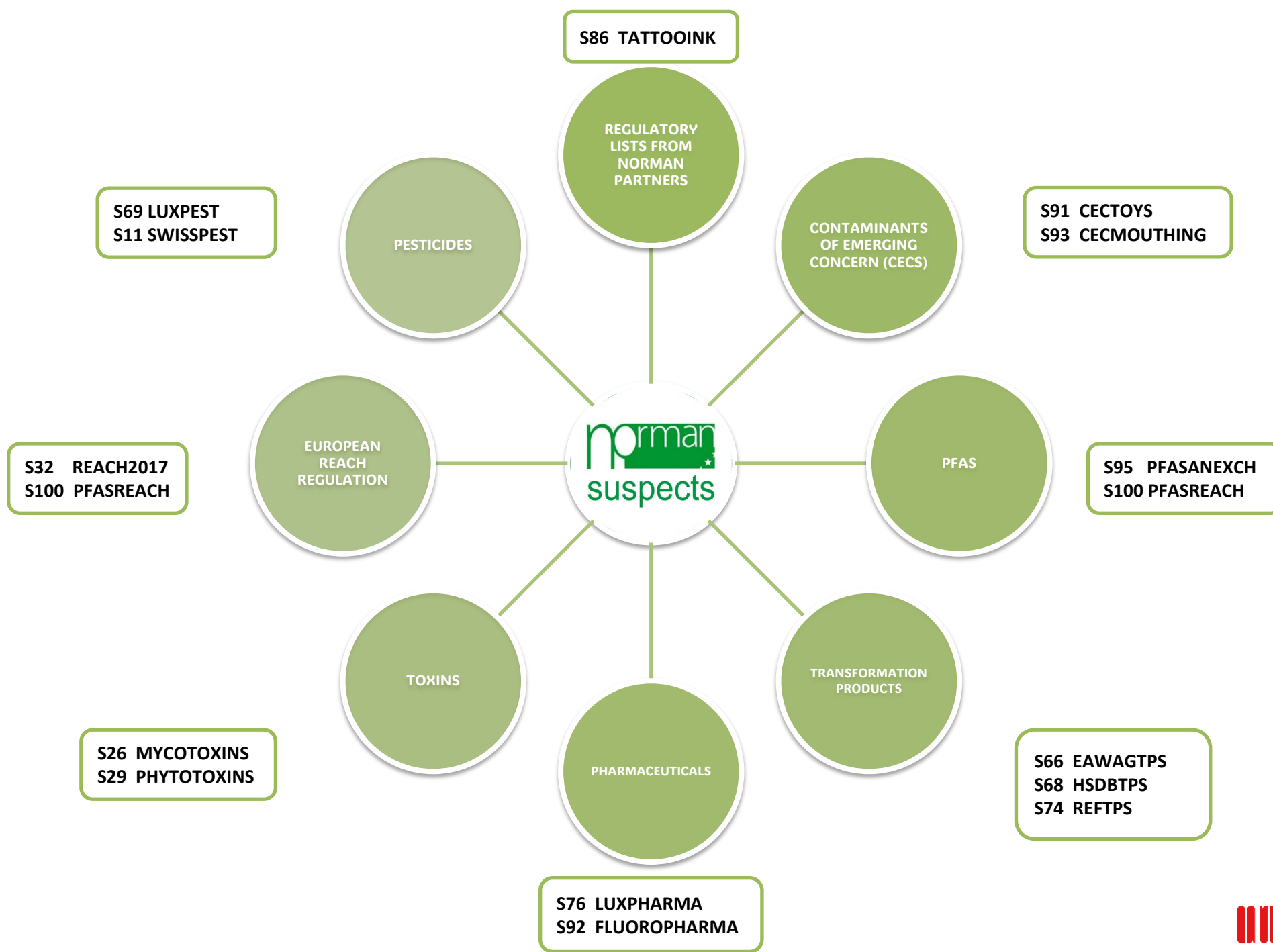
NORMAN-SLE in PubChem



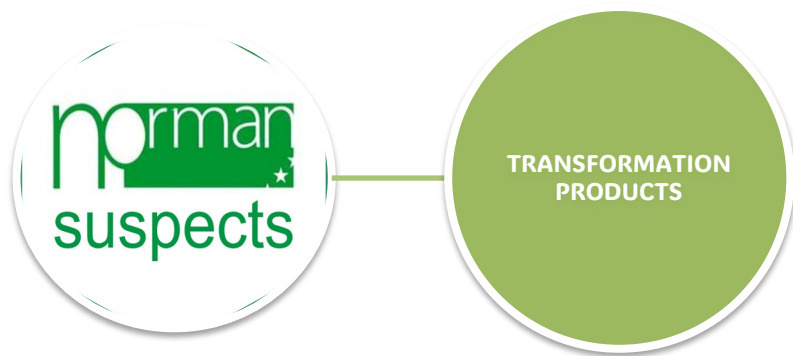
The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. The NORMAN Suspect List Exchange (NORMAN-SLE) is a central access point to find suspect lists relevant for various environmental monitoring questions, described in DOI:10.1186/s12302-022-00680-6

Organization	NORMAN Network (c/o UniLu)
Category	Research and Development
URL	https://www.norman-network.com/nds/SLE/
License Note	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
License URL	https://creativecommons.org/licenses/by/4.0/
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, 4367
Data Source ID	23819
Data in PubChem	118,557 Live Substances 22,335 Annotations 1 Classification
Last Updated	2023/10/09

▼ NORMAN Suspect List Exchange Classification	?	↗	115,725
▶ S13 EUCOSMETICS Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006)	?		3,955
▶ S25 OECDPFAS List of PFAS from the OECD	?		3,678
▶ S36 UBAPMT Potential Persistent, Mobile and Toxic (PMT) substances	?		254
▶ S47 ECHAPLASTICS A list from the Plastic Additives Initiative Mapping Exercise by ECHA	?		241
▶ S50 CCSCOMPEND The Unified Collision Cross Section (CCS) Compendium	?		869
▶ S60 SWISSPEST19 Swiss Pesticides and Metabolites from Kiefer et al 2019	?		1,359
▶ S61 UJCCSLIB Collision Cross Section (CCS) Library from UJI	?		574
▶ S66 EAWAGTPS Parent-Transformation Product Pairs from Eawag	?		258
▶ S68 HSDBTPS Transformation Products Extracted from HSDB Content in PubChem	?		740
▶ S69 LUXPEST Pesticide Screening List for Luxembourg	?		386
▶ S72 NTUPHTW Pharmaceutically Active Substances from National Taiwan University	?		1,068
▶ S75 CyanoMetDB Comprehensive database of secondary metabolites from cyanobacteria	?		2,553
▶ S77 FCCDB Food Contact Chemicals Database v5.0	?		5,989
▶ S79 UACCSCEC Collision Cross Section (CCS) Library from UAntwerp	?		148
▶ S80 PFASGLUEGE Overview of PFAS Uses	?		1,251



Why SLE ?



S66 EAWAGTPS
S68 HSDBTPS
S74 REFTPS

HERBICIDE

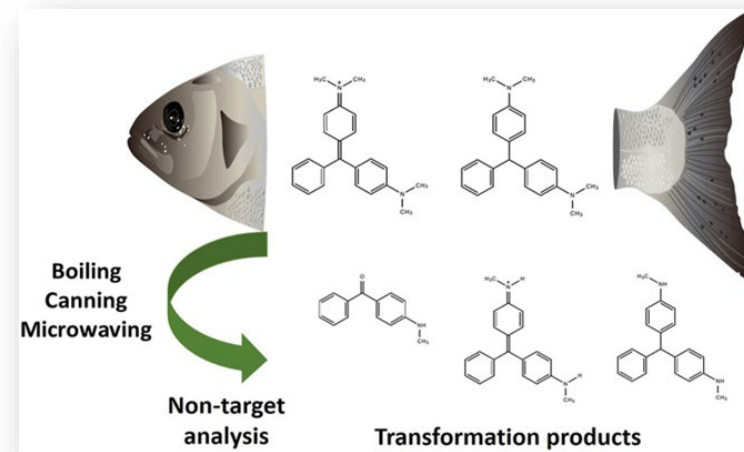
PubChem Terbutylazine-2-hydroxy (Compound)

8.1 Transformations

Page 2 of 9 items View More Rows & Details Download

SORT BY Please Choose One

Predecessor Image	Predecessor Name	Transformation	Successor Image	Successor Name	Enzyme
	Terbutryn	Oxidation		Terbutylazine-2-hydroxy	
	Terbutylazine	Dehalogenation		Terbutylazine-2-hydroxy	
	Terbutylazine-2-hydroxy	Deethylation		Terbutylazine-desethyl-2-hydroxy	



Baesu et al. (2021) DOI: [10.1016/j.crfs.2021.09.010](https://doi.org/10.1016/j.crfs.2021.09.010).



FAIR Transformations in PubChem and NORMAN-SLE



NORMAN SLE : Take Home Messages



Acknowledgements



RESEARCH

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The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

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